

Cooling classical particles with a microcanonical Szilard engine

Rahul Marathe* and J. M. R. Parrondo†

*Departamento de Física Atómica, Molecular y Nuclear and GISC,
Universidad Complutense de Madrid, 28040-Madrid, Spain*

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The possibility of extraction of energy from a system in a cyclic process is discussed. We present an explicit example where a system, initially prepared in a microcanonical state, is able to perform such operation. The example is similar to the Szilard engine, but the microcanonical initial condition allows one to design a protocol where measurement is not necessary.

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Extracting energy from a system faces limitations imposed by Thermodynamics and Statistical Mechanics. Kelvin statement of the Second Law precludes the cyclic extraction of energy from a single thermal bath. Using Hamiltonian dynamics, Jarzynski [1] proved that this is the case for systems initially prepared in a Boltzmann state. Suppose a system described by a Hamiltonian $H(q, p; \lambda_1, \dots, \lambda_n)$, where (q, p) stands for a point in the phase space and $\lambda_1(t), \dots, \lambda_n(t)$ are external parameters operated by an external agent. The system is isolated, except for the interaction with this external agent, and consequently the probability density $\rho(q, p; t)$ obeys the time-dependent Liouville equation. Jarzynski [1] proved that, along an arbitrary cyclic process $\lambda_i(0) = \lambda_i(\tau)$, the average energy of the system necessarily increases, i.e., cyclic energy extraction is not possible. Campisi [2] further generalized this result proving that the extraction is impossible for any initial distribution $\rho(q, p; 0)$, such that the resulting probability density for the energy is a decreasing function. Both Jarzynski's and Campisi's results can be considered as mechanical proofs of the Kelvin statement of the Second Law.

On the other hand, the microcanonical distribution, where the total energy of the system is known with a given accuracy, does not fulfill Campisi's requirement. In fact, Sato [3] devised a particular example—a one-dimensional particle in a potential depending on one parameter $\lambda(t)$ —where, starting in a microcanonical state, the energy of the particle decreases along a process with $\lambda(0) = \lambda(\tau)$. Although this result is remarkable, the extraction of energy cannot be repeated, since after the first cycle the probability density is no longer microcanonical.

In this Letter we present an explicit example where energy can be extracted in a systematic way. It is a microcanonical version of the Szilard engine [4], consisting of a classical particle in a time-dependent potential. In contrast with the original Szilard model, the microcanonical initial condition allows one to operate the engine with-

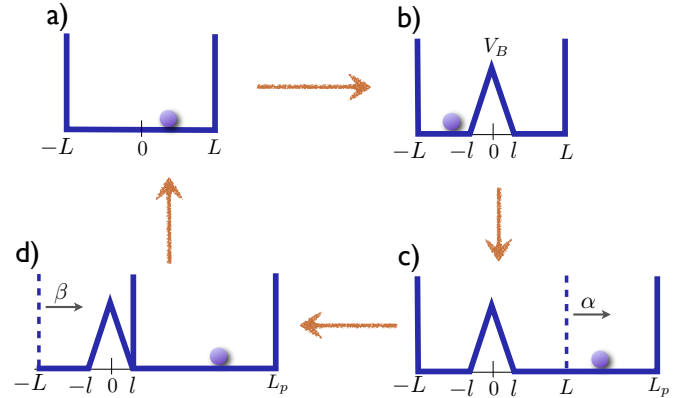


FIG. 1: (color online). Different steps in the microcanonical Szilard engine. At stage (b), we have plotted the particle in the left half but recall that, under the protocol described in the text, the particle may have enough energy to move all over the whole box.

out measurements. Our example provides a new strategy for microscopic cooling of classical isolated particles, but also touches some fundamental issues regarding the mechanical rationale of the Second Law.

Our microcanonical version of the Szilard engine [4] consists of a single one-dimensional isolated particle of mass m in a potential modified by an external agent. The particle is initially confined in a box of length $2L$ and the potential is changed as shown in Fig. 1. In (a–b), a barrier is raised at the center of the box up to height V_B at speed γ . The barrier potential is given by:

$$V(x; t) = \begin{cases} \frac{\gamma t}{l} (l - |x|) & |x| \leq l \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

for $t \in [0, V_B/\gamma]$. In the second step (b–c), the right wall is moved from L to $L_p = 2L + l$ with velocity α . Finally, along (c–d), the left wall is moved from $-L$ to l , with velocity β and the potential recovers its initial configuration (but shifted to the right).

*Electronic address: rahul@fis.ucm.es

†Electronic address: parrondo@fis.ucm.es

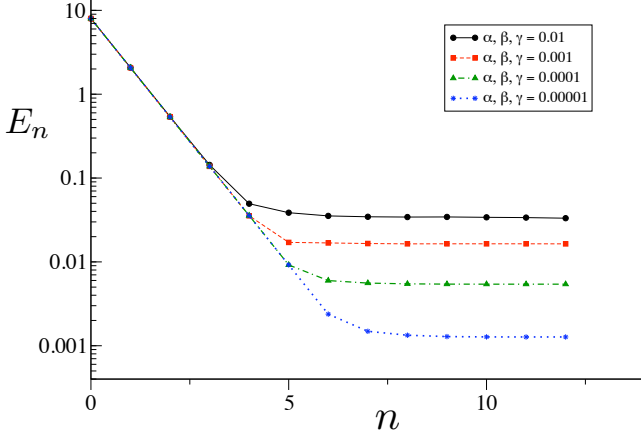


FIG. 2: (color online). Log-linear plot of the energy E_n versus the cycle number n . Parameters used are $m = 1$, $L = 20$, $l = 1.0$, for different values of α, β, γ . The maximum height of the barrier in cycle n is $V_B^{(n)} = \kappa^n E_0$, with $\kappa = [1/2 + l/(6L)]^2$.

Now suppose that the barrier height V_B is equal to the initial energy of the particle E_0 . When the barrier is raised along step (a–b), the particle gains some small amount of energy, and then the barrier is not high enough to confine the particle in one of the halves of the container. Along the expansion (b–c), the particle loses energy in each collision with the right moving wall (in each collision the velocity changes from v to $-v + 2\alpha$). After a certain number of collisions, its energy drops below V_B and the particle gets confined in the rightmost half of the container. As a consequence, the final compression (c–d) does not affect the particle much and the net effect of the process is a reduction of its energy. Since the particle will be *always* confined in the rightmost half of the box, no measurement is necessary along the step (b–c), unlike the original Szilard engine. This situation is possible only for certain values of V_B depending on the initial energy of the particle, although not on its position. We can therefore design a protocol that works for microcanonical initial conditions: fixed energy (velocity) and random position inside the box. Moreover, if the above steps are carried out quasi-statically, the energy change is deterministic. Then, by taking the appropriate values of V_B in each cycle, we can systematically extract energy at least down to a certain value which can be made arbitrarily small by reducing the speeds α, β , and γ . Fig. 2 shows the energy after each cycle, following the described protocol, for different values of α, β, γ . Data presented in Fig. 2 have been obtained by an event driving algorithm and solving exactly the Newton’s equations for the motion of the particle. Along step (a–b), a third order polynomial must be solved for the motion along the barrier.

For a full understanding of our microcanonical Szilard engine, it is convenient to study in detail the quasi-static limit, $\alpha, \beta, \gamma \rightarrow 0$. Consider a point (x_0, p_0) in phase

space, with position x_0 , momentum p_0 , and energy $E_0 \equiv H(x_0, p_0; 0) = p_0^2/(2m) + V(x_0; 0)$, evolving as $(x(t), p(t))$ with energy $E(t) = H(x(t), p(t); t)$. The action

$$\phi_t(E(t)) \equiv \int_{H(x,p;t) < E(t)} dx dp \quad (2)$$

is an *adiabatic invariant*, i.e., is constant for quasi-static changes of the Hamiltonian [5, 6]. In our case, the initial action $\phi_0 = 4L\sqrt{2mE_0}$ would in principle remain constant along the cycle. However, the invariance has an exception: when an orbit changes abruptly due to segregation, confinement or sudden expansion, induced by the barrier, the action changes accordingly [6, 7]. Below we derive the conditions determining these changes.

For a generic height V of the barrier and location of the left (L_l) and right (L_r) walls, the action of an orbit with energy E reads:

$$\phi(E) = \begin{cases} \sqrt{2mE} \left(2(L_{l,r} - l) + \frac{4lE}{3V} \right) & \text{if } E < V \\ \sqrt{2mE} \left\{ 2(L_r + L_l - 2l) + \frac{8lE}{3V} \left[1 - (1 - V/E)^{3/2} \right] \right\} & \text{if } E > V \end{cases} \quad (3)$$

where L_r or L_l in the first line is taken depending on the side of the box where the orbit is confined. The discontinuity of the action $\phi(E)$ given by Eq. (3) at $E = V$ is a trademark of the breaking of its invariance. Suppose that the barrier is high enough to split, at some stage of step (a–b), the orbit of a particle with initial energy E_0 . Right before the segregation, the energy E_{seg} of the particle is equal to the height V of the barrier. Setting $E = V$ in Eq. (3) for $E > V$, the invariance for the action (right before segregation) implies:

$$\sqrt{2mE_{\text{seg}}} \left[4(L - l) + \frac{8l}{3} \right] = 4L\sqrt{2mE_0} \quad (4)$$

Segregation actually occurs if the maximum height V_B is greater than E_{seg} , i.e., if

$$E_0 < \left(1 - \frac{l}{3L} \right)^2 V_B \quad (5)$$

Segregation decreases the action of individual orbits by

$$\Delta\phi_{\text{seg}} = -\phi_0/2 = -2L\sqrt{2mE_0} \quad (6)$$

Orbits lying in the right side of the box do not suffer any further collapse or expansion. On the other hand, those in the left hand undergo a sudden expansion when reaching an energy V_B along step (d–a). The increase of the action equals the action corresponding to a new lobe added to the orbit in the right side, which is given by the

right contribution in (3) at $E = V = V_B$ ($E < V$) and $L_r = 2L + l$, yielding:

$$\Delta\phi_{\text{exp}} = 4\sqrt{2mV_B} \left(L + \frac{l}{3} \right). \quad (7)$$

If there is no segregation, i.e., if the particle reaches stage (b) with an energy greater than V_B , then along step (b-c) the energy of the particle decreases, due to collisions with the right moving wall, and eventually can reach the critical value V_B confining the particle in the rightmost half of the container. In this case, the orbit of the particle suddenly loses the left lobe (see Fig. 5). Before the confinement, the action is invariant. Setting $E = V = V_B$, $L_l = L$ in Eq. (3) for $E > V$, the invariance for the action, right before confinement, reads:

$$\sqrt{2mV_B} \left[2(L_{\text{conf}} + L - 2l) + \frac{8l}{3} \right] = 4L\sqrt{2mE_0}. \quad (8)$$

We have written $L_r = L_{\text{conf}}$, the position of the right wall in the moment of confinement, which is at most $L_p = 2L + l$. Therefore, confinement occurs if:

$$\sqrt{2mV_B} \left[2(3L - l) + \frac{8l}{3} \right] > 4L\sqrt{2mE_0}. \quad (9)$$

Thus Eq. (5) and Eq. (9), constitute the condition for the confinement given by:

$$\left(1 - \frac{l}{3L} \right)^2 V_B < E_0 < \left(\frac{3}{2} + \frac{l}{6L} \right)^2 V_B. \quad (10)$$

The change in the action due to confinement is the action corresponding to the left branch of the orbit disappearing after confinement, which is given by the left contribution in (3) at $E = V = V_B$ ($E < V$) and $L_l = L$, yielding:

$$\Delta\phi_{\text{conf}} = -\sqrt{2mV_B} \left(2L - \frac{2l}{3} \right). \quad (11)$$

Finally, if the initial energy is large, $E_0 > [3/2 + l/(6L)]^2 V_B$, the orbit spans all over the box along the whole process and the action is invariant. Summarizing, the final action is

$$\phi_f = \phi_0 + \Delta\phi, \quad (12)$$

with $\Delta\phi = \Delta\phi_{\text{conf}} < 0$ if Eq. (10) is satisfied, $\Delta\phi = 0$ if the energy is above the upper limit in Eq. (10), and $\Delta\phi = \Delta\phi_{\text{seg}} < 0$ or $\Delta\phi = \Delta\phi_{\text{seg}} + \Delta\phi_{\text{exp}} > 0$ if it is below the lower limit. These two values are taken with probability 1/2, respectively. We can now calculate the final energy E_f since $\phi_f = \phi_0 + \Delta\phi = 4L\sqrt{2mE_f}$, yielding

$$E_f = \left(\sqrt{E_0} + \frac{\Delta\phi}{4L\sqrt{2m}} \right)^2. \quad (13)$$

Fig. 3 shows the final energy as a function of the ini-

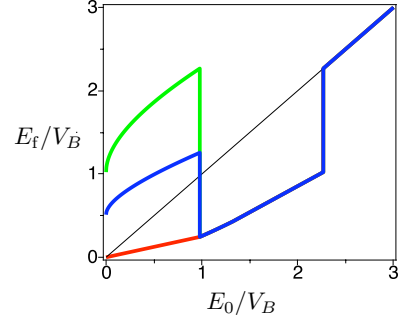


FIG. 3: (color online). Final energy as a function of the initial energy in the quasistatic limit, as given by (13). Parameters used are $m = 1$, $L = 20$, $l = 1.0$. For small initial energies, particles are segregated to the left or right half of the box at step (a-b) with probability 1/2 corresponding, respectively, to the green and red curves depicted in the figure. The blue curve is the average final energy.

tial energy. We see that the extraction of energy is only possible in the window defined by Eq. (10). However, since the energy change in the quasi-static limit is deterministic (if there is no segregation) we can tune V_B to verify Eq. (10) in subsequent cycles. The simplest choice is to set the height of the barrier at cycle n , $V_B^{(n)}$, equal to the energy of the particle when the cycle starts. In the case $V_B = E_0$, the final energy after a cycle reads $E_f = \kappa E_0$ with $\kappa = [1/2 + l/(6L)]^2$. Therefore, an appropriate choice is $V_B^{(n)} = \kappa^n E_0$, which is the protocol followed in Fig. 2. Notice that this choice is made *a priori* and does not depend on the actual evolution of the system. Consequently, for finite velocities α, β, γ the protocol fails, since the energy does not follow a deterministic sequence as we depart from the quasi-static limit. However, the energy at which the protocol starts to fail can be made arbitrarily small by reducing the speed of the process, as Fig. 2 indicates.

Our example prompts a crucial question: is the possibility of extraction of energy a special feature of one dimensional systems or can be extended to systems with several degrees of freedom? A naive extension of the microcanonical Szilard engine to two or more independent particles does not allow the systematic extraction of energy. Consider two one-dimensional particles confined in the interval $[-L, L]$. They are independent except for the initial preparation in a microcanonical state with total energy E_0 , $\rho_{E_0}(p_1, p_2; 0) = \delta(E_0 - p_1^2/2m - p_2^2/2m) / (2\pi m)$. For simplicity, we will assume that the potential only affects particle 1. Then we can apply the above results using as initial distribution of energy the corresponding distribution of the energy of particle 1:

$$\begin{aligned} \rho(E; 0) &= \int dp_1 dp_2 \delta\left(E - \frac{p_1^2}{2m}\right) \rho_{E_0}(p_1, p_2; 0) \\ &= \frac{1}{\pi \sqrt{E(E_0 - E)}} \end{aligned} \quad (14)$$

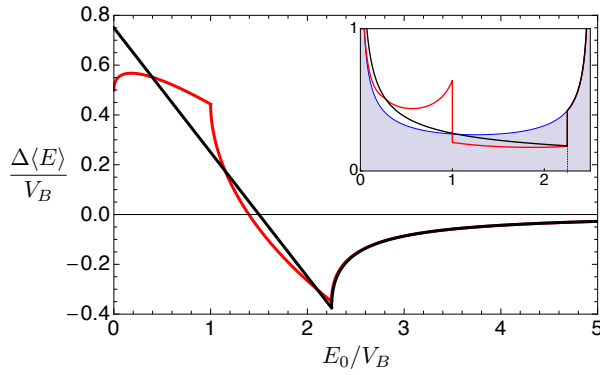


FIG. 4: (color online). Average change of energy after one (red) and an infinite number (black) of repetitions of the protocol with fixed V_B and $l = 0$ for two particles, as a function of the initial total energy E_0 . Inset: probability distribution of the energy of the particle undergoing the protocol initially (filled blue), after one (red) and an infinite number of repetitions (black) for $V_B = 1$ and $E_0 = 2.5$.

Fig. 4 shows the change of energy for an infinitely narrow barrier $l = 0$, as a function of E_0/V_B . The red curve corresponds to the change after one run of the protocol. One can extract energy in a single run for $E_0 \geq 1.4V_B$, but the probability distribution of the energy of particle 1 changes in a rather uncontrolled way (see inset of Fig. 4, red curve), and a repetition of the protocol does not further decrease the energy. The black curve in Fig. 4 shows the change of energy after an infinite number of cycles (with the same V_B). Adaptive protocols changing V_B in each cycle can slightly improve the energy decrease, but the systematic extraction of energy seems impossible in the case of two particles. With three or more particles, the probability distribution of the energy of particle 1 is a decreasing function and, following Campisi's theorem [2], the energy increases even after the first run of the protocol.

However, the basic mechanism of our microcanonical Szilard engine is a “shuffling” of the phase space that could in principle work in systems with several degrees of freedom. Fig. 5 shows how the phase space changes after one run of the protocol for $l = 0$ and a single one-dimensional particle. Points with energy below V_B (striped regions) are mapped to two regions of half size; those with energy between V_B and $9V_B/4$ (blue regions) shift down, whereas the rest are not affected by the protocol. Notice that this shuffling is fully compatible with Liouville theorem: the volume of any subset in the phase space is conserved. On the other hand, it needs the collapse or split of orbits. Otherwise, the adiabatic invariance of the volume enclosed by an energy shell implies that every point in the phase space goes back to its initial position after any quasistatic cycle.

Up to our knowledge, there is no fundamental obstacle

to reproduce this shuffling of the phase space in a system with many degrees of freedom. It is an open question to find an explicit example (probably more involved than a naive generalization of our protocol) or, on the contrary, to prove that the phenomenon described in this Letter is exclusive to systems with one degree of freedom. Either one or the other, the answer to this question touches a fundamental problem: the mechanical rationale of the Kelvin statement of the Second Law for systems prepared in the microcanonical state. Let us finally recall that the microcanonical ensemble, although of limited use in real applications, is essential for an objective formulation of Statistical Mechanics [8, 9].

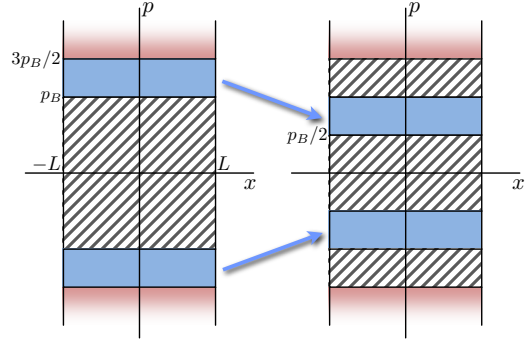


FIG. 5: (color online). Evolution of regions in phase space after completing the protocol with a barrier height V_B and $l = 0$, for a single one-dimensional particle. The striped region with energy lower than V_B , $p \in [-p_B, p_B]$, with $p_B = \sqrt{2mV_B}$, splits into three regions leaving room to the blue region $p \in [p_B, 3p_B/2]$ to move down to $p \in [p_B/2, p_B]$.

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